

201-16221A

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L100 C100

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C*****
C
C Import/Export - File for the
C
C International Uniform Chemical Information Database
C
C Column 1- 4: Blocknumber / Fieldnumber
C Column 6-80: Blockname / Fieldvalue
C Date : 27-DEC-2005 15:01:27
C Company : Arcadis 27713 Durham, NC
C*****
C
V IUCLID-Export V4.00
C
CS ISO-Latin 1
C
NL GBR
C
B005 SUBST_MASTER_TAB
F001 102-60-3
F002 Y26-001
EOB
C
B006 SUBST_IDENT_TAB
F001 102-60-3
F002 Y28-001
F003 Y27-001
F004 102-60-3
F005 1
EOR
F001 102-60-3
F002 Y28-002
F003 Y27-017
F004 Quadrol
F005 2
F006 ENG
EOR
F001 102-60-3
F002 Y28-003
F003 Y27-003
F004 C14 H32 N2 O4
F005 3
EOR
F001 102-60-3
F002 Y28-001
F003 Y27-005
F004 292.42
F005 4
EOR
F001 102-60-3
F002 Y28-002
F003 Y27-016
F004 N,N,N',N'-tetrakis(2-hydroxypropyl)ethylenediamine
F005 5
F006 ENG
EOB
C
```

B003 DS_ADMIN_TAB

F002 4

F001 102-60-3

F009 N

F005 11030761

F006 20-09-2003

F007 11030761

F008 20-09-2003

F003 09-12-2005

F102 A35-01

EOB

C

B004 COMPANY_TAB

F001 11030761

F003 Arcadis

F004 4915 Prospectus Drive, Suite F

F005 Durham, NC

F006 27713

F008 A31-024

EOB

C

C ***** NEW DATA SET *****

C

D 4

C

B052 DS_COMPONENT_JOIN_TAB

F001 4

F002 0

F003 1.0.1

F004 1

F005 1

F006 16-10-2003

F007 01-10-2003

EOR

F001 4

F002 0

F003 1.1.0

F004 1

F005 1

F006 29-09-2003

F007 29-09-2003

EOR

F001 4

F002 0

F003 1.1.1

F004 1

F005 1

F006 02-10-2003

F007 29-09-2003

EOR

F001 4

F002 0

F003 1.2

F004 1

F005 1

F006 02-10-2003

F007 29-09-2003

EOR
F001 4
F002 0
F003 1.2
F004 2
F005 2
F006 01-10-2003
F007 29-09-2003
EOR
F001 4
F002 0
F003 1.2
F004 3
F005 3
F006 29-09-2003
F007 29-09-2003
EOR
F001 4
F002 0
F003 1.2
F004 4
F005 4
F006 01-10-2003
F007 01-10-2003
EOR
F001 4
F002 0
F003 1.2
F004 5
F005 5
F006 01-10-2003
F007 01-10-2003
EOR
F001 4
F002 0
F003 1.2
F004 6
F005 6
F006 01-10-2003
F007 01-10-2003
EOR
F001 4
F002 0
F003 1.8.6
F004 1
F005 1
F006 01-10-2003
F007 29-09-2003
EOR
F001 4
F002 0
F003 2.1
F004 1
F005 1
F006 09-12-2005
F007 29-09-2003
EOR

F001 4
F002 0
F003 2.2
F004 1
F005 1
F006 09-12-2005
F007 29-09-2003
EOR
F001 4
F002 0
F003 2.3
F004 1
F005 1
F006 29-09-2003
F007 29-09-2003
EOR
F001 4
F002 0
F003 2.4
F004 1
F005 1
F006 14-10-2003
F007 01-10-2003
EOR
F001 4
F002 0
F003 2.5
F004 1
F005 1
F006 13-10-2003
F007 01-10-2003
EOR
F001 4
F002 0
F003 2.6.1
F004 1
F005 1
F006 01-12-2003
F007 01-10-2003
EOR
F001 4
F002 0
F003 3.1.1
F004 1
F005 1
F006 14-10-2003
F007 02-10-2003
EOR
F001 4
F002 0
F003 3.1.2
F004 2
F005 2
F006 21-06-2004
F007 21-06-2004
EOR
F001 4

F002 0
F003 3.3.2
F004 1
F005 1
F006 09-12-2005
F007 07-10-2003
EOR
F001 4
F002 0
F003 3.5
F004 2
F005 2
F006 09-12-2005
F007 05-12-2005
EOR
F001 4
F002 0
F003 3.5
F004 3
F005 3
F006 09-12-2005
F007 05-12-2005
EOR
F001 4
F002 0
F003 4.1
F004 2
F005 2
F006 21-06-2004
F007 14-10-2003
EOR
F001 4
F002 0
F003 4.2
F004 1
F005 1
F006 21-06-2004
F007 02-10-2003
EOR
F001 4
F002 0
F003 4.3
F004 1
F005 1
F006 21-06-2004
F007 02-10-2003
EOR
F001 4
F002 0
F003 5.1.1
F004 1
F005 1
F006 14-10-2003
F007 01-10-2003
EOR
F001 4
F002 0

F003 5.4
F004 2
F005 2
F006 14-10-2003
F007 07-10-2003

EOB

F001 4
F002 0
F003 5.5

F004 1
F005 1
F006 14-10-2003
F007 01-10-2003

EOB

C

B051 DS_COMPONENT_TAB

F001 4
F002 0
F003 102-60-3

F012 N
F010 29-09-2003
F004 11030761
F005 20-09-2003
F006 11030761
F007 20-09-2003
F009 A35-01

EOB

C

B115 GI_COMPANY_TAB

F001 4
F002 1
F003 16-10-2003
F004 IUC4
F007 A34-03
F008 Arcadis
F009 4915 Prospectus Drive, Suite F
F010 Durham, NC
F011 27713
F013 A31-024
F014 919-544-4535
F018 Jane Staveley
F022 jstaveley@arcadis-us.com
F023 www.arcadis-us.com

EOB

C

B007 GI_SUBSTANCE_TAB

F001 4
F002 1
F003 29-09-2003
F004 IUC4
F008 C14 H32 N2 O4
F009 292.42

EOB

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B101 GI_GENERAL_INFORM_TAB

F001 4
F002 1

F003 02-10-2003

F004 IUC4

F007 A02-03

F008 100

F010 A04-04

F011 A19-02

F015 white

F016 mild polyol

F017 C51-001

EOB

C

B102 GI_SYNONYM_TAB

F001 4

F002 1

F003 02-10-2003

F004 IUC4

F007 Tetrahydroxypropyl Ethylenediamine

EOR

F001 4

F002 2

F003 01-10-2003

F004 IUC4

F007 1,1',1'',1'''-(1,2-ethanediylldinitrilo)tetrakis-2-propanol.

EOR

F001 4

F002 3

F003 29-09-2003

F004 IUC4

F007 Edetol

EOR

F001 4

F002 4

F003 01-10-2003

F004 IUC4

F007 N,N,N',N'- tetrakis(2-hydroxylpropyl)ethylenediamine

EOR

F001 4

F002 5

F003 01-10-2003

F004 IUC4

F007 Entprol

EOR

F001 4

F002 6

F003 01-10-2003

F004 IUC4

F007 2-propanol, 1,1',1'',1'''-(1,2-ethanediylldinitrilo)tetrakis-

EOB

C

B127 GI_INTERNAL_REF_TAB

F001 4

F002 1

F003 01-10-2003

F004 IUC4

F007 A47-002

F008 listed on inventory

EOB

C

B201 PC_MELTING_TAB

F001 4

F002 1

F003 09-12-2005

F004 IUC4

F015 A36-002

F010 A30-03

F012 P01-04

F013 2005

F014 A03-03

F017 A02-06

F018 130

F020 A01-03

EOB

C

B202 PC_BOILING_TAB

F001 4

F002 1

F003 09-12-2005

F004 IUC4

F016 A36-002

F011 P02-01

F013 P03-04

F014 2005

F015 A03-03

F018 A01-03

EOB

C

B203 PC_DENSITY_TAB

F001 4

F002 1

F003 29-09-2003

F004 IUC4

F007 P05-03

F008 A02-03

F009 1.013

EOB

C

B204 PC_VAPOUR_TAB

F001 4

F002 1

F003 14-10-2003

F004 IUC4

F015 A36-002

F007 A02-03

F008 .000000012

F010 P02-01

F012 P06-03: Modified Grain Method

EOB

C

B205 PC_PARTITION_TAB

F001 4

F002 1

F003 13-10-2003

F004 IUC4

F014 A36-002

F007 A02-03
F008 -2.08
F011 P07-04
F020 C15-001

EOB

C

B206 PC_WATER_SOL_TAB

F001 4

F002 1

F003 01-12-2003

F004 IUC4

F023 A36-003

F007 A02-05

F008 P08-01

F009 1000

F011 25

F030 C14-001

EOB

C

B301 EN_PHOTODEGRADATION_TAB

F001 4

F002 1

F003 14-10-2003

F004 IUC4

F045 A36-002

F008 F01-01

F009 F02-05

F034 F06-03

F044 A02-03

F037 .0000000002307401

F038 A02-03

F040 50

F041 .6

F042 F05-02

EOB

C

B302 EN_STABILITY_IN_WATER_TAB

F001 4

F002 2

F003 21-06-2004

F004 IUC4

F008 F08-01

EOB

C

B306 EN_DISTRIBUTION_TAB

F001 4

F002 1

F003 09-12-2005

F004 IUC4

F010 A36-002

F007 F24-02

F008 F23-03

EOB

C

B308 EN_BIODEGRADATION_TAB

F001 4

F002 2

F003 09-12-2005
F004 IUC4
F047 A36-002
F007 A01-03
F008 F25-01
F009 F26-14
F010 2005
F011 F27-0137
F012 35
F013 F28-02
F014 F29-03
F015 A02-03
F016 20
F017 10
F018 28
F019 F05-01
F020 F30-02: not readily biodegradable according to OECD criteria
F021 A02-03
F022 20
F023 10
F024 28
F025 F31-01
F026 A02-03
F027 50
F028 40
F029 42
F030 F31-01
F056 A02-03
F057 100
F058 90
F059 14
F060 F31-01
F046 A03-03
F049 20
F050 F28-02
F051 F29-02
F052 42
F053 F05-01
F066 E36-001
EOR
F001 4
F002 3
F003 09-12-2005
F004 IUC4
F047 A36-002
F007 A01-03
F008 F25-01
F009 F26-25: Directive 88/302/EEC, C.11: Biodegradation: activated sludge
* respiration inhibition test
F010 2005
F011 F27-0137
F012 1000
F013 F28-02
F014 F29-03
F046 A03-03
F052 30
F053 F05-03

F066 E36-007: 3,5-dichlorophenol

EOB

C

B401 EC_FISHTOX_TAB

F001 4

F002 2

F003 21-06-2004

F004 IUC4

F033 A36-003

F007 A01-03

F008 E01-05

F009 E02-0119

F011 1976

F012 96

F013 E04-02

F014 E05-02

F027 TLm

F028 A02-04

F029 1000

F031 A03-01

F032 A03-01

F035 TL1

F036 A02-04

F037 1000

F039 TL99

F040 A02-04

F041 1000

EOB

C

B402 EC_DAPHNIATOX_TAB

F001 4

F002 1

F003 21-06-2004

F004 IUC4

F032 A36-002

F008 E06-0013

F009 E07-04: calculated

F011 48

F012 E04-02

F013 E05-02

F020 A02-03

F021 1435

F042 E01-03: calculated

F045 E35-01

EOB

C

B403 EC_ALGAETOX_TAB

F001 4

F002 1

F003 21-06-2004

F004 IUC4

F036 A36-002

F008 E08-0063: green algae

F009 E09-04: calculated

F012 96

F013 E04-02

F014 E05-02

F027 A02-03

F028 662

F030 ChV

F031 A02-03

F032 57.7

F050 E35-01

F051 E35-01

EOB

C

B501 TO_ACUTE_ORAL_TAB

F001 4

F002 1

F003 14-10-2003

F004 IUC4

F017 A36-003

F008 T01-03

F009 T02-24

F010 T03-03: study pre-dates standardized methods

F011 1956

F012 A02-03

F013 11200

F015 T04-01

F016 A03-01

F019 T24-02

F020 10

F021 T52-007

F023 4400, 5600, 7500, 9750, 12600, 16500 mg Quadrol/kg

EOB

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B508 TO_REPEATED_DOSE_TAB

F001 4

F002 2

F003 14-10-2003

F004 IUC4

F030 A36-003

F008 T02-24

F009 T23-48: Harlan albino

F010 T24-03

F011 T25-09

F013 1956

F014 three months

F015 ad libitum

F016 no post-exposure observation period

F017 Doses were equivalent to average daily intakes of 70, 210, 720, 2170 and

* 3750 mg/kg bw

F018 T27-04

F019 A02-06

F020 600

F021 900

F022 T28-02

F029 A03-01

F032 C07-001

EOB

C

B509 TO_GENETIC_IN_VITRO_TAB

F001 4

F002 1

F003 14-10-2003
F004 IUC4
F016 A36-005
F007 A01-02
F008 T30-01
F009 T31-18: only referred to as "standard plate"
F010 1994
F011 Salmonella typhimurium TA97, TA98, TA100, TA 102; E. coli WP2(PKM101)
F012 T32-03
F013 T33-02
F014 A03-02
F015 200 - 10000 ug/plate (test material solvent: DMSO)
EOB
C
B601 TEXT_TAB
F002 4
F010 1.0.1
F004 1
F005 RM
F006 This document has been prepared on behalf of BASF Corporation
F007 This document has been prepared on behalf of BASF Corporation
F020 725
EOR
F002 4
F010 1.1.1
F004 1
F005 RE
F006 MSDS, BASF Corp., 17 SEP 2002
F007 MSDS, BASF Corp., 17 SEP 2002
F020 227
EOR
F002 4
F010 1.2
F004 1
F005 RE
F006 MSDS, BASF Corp., 17 SEP 2002
F007 MSDS, BASF Corp., 17 SEP 2002
F020 228
EOR
F002 4
F010 1.2
F004 2
F005 RE
F006 MSDS, MDL Information Systems, 11 DEC 2001
F007 MSDS, MDL Information Systems, 11 DEC 2001
F020 229
EOR
F002 4
F010 1.2
F004 3
F005 RE
F006 MSDS, MDL Information Systems, 22 MAR 2001
F007 MSDS, MDL Information Systems, 22 MAR 2001
F020 230
EOR
F002 4
F010 1.2

F004 4
F005 RE
F006 MSDS, BASF Corp., 17 SEP 2002
F007 MSDS, BASF Corp., 17 SEP 2002
F020 395
EOR
F002 4
F010 1.2
F004 5
F005 RE
F006 MSDS, MDL Information Systems, 11 DEC 2001
F007 MSDS, MDL Information Systems, 11 DEC 2001
F020 396
EOR
F002 4
F010 1.2
F004 6
F005 RE
F006 MSDS, MDL Information Systems, 11 DEC 2001
F007 MSDS, MDL Information Systems, 11 DEC 2001
F020 397
EOR
F002 4
F010 2.1
F004 1
F005 ME
F006 Melting temperature was measured by Differential Scanning Calorimetry. A
* preliminary test was run between -100 degrees C and +400 degrees C.
F007 Melting temperature was measured by Differential Scanning Calorimetry. A
* preliminary test was run between -100 degrees C and +400 degrees C.
F020 868
EOR
F002 4
F010 2.1
F004 1
F005 RE
F006 BASF, Final Report, Physico-chemical properties of "Quadrol Polyol",
* Study No. 05L00061, GKA Competence Center Analytics, June, 2005.
F007 BASF, Final Report, Physico-chemical properties of "Quadrol Polyol",
* Study No. 05L00061, GKA Competence Center Analytics, June, 2005.
F020 399
EOR
F002 4
F010 2.1
F004 1
F005 RS
F006 No melting temperature could be observed in the temperature range of
** -100 degrees C to +40 degrees C even with the addition of aluminum oxide
* as a crystallization aid. A glass transition was observed with a
* half-step temperature of -31.5 d.
F007 No melting temperature could be observed in the temperature range of
** -100 degrees C to +40 degrees C even with the addition of aluminum oxide
* as a crystallization aid. A glass transition was observed with a
* half-step temperature of -31.5 degrees C.
F020 869
EOR
F002 4

F010 2.1
F004 1
F005 TS
F006 Quadrol Polyol, Batch No. WPYY-520B; produced Feb 04, 2003, purity
* unknown, stored at ambient temperature under nitrogen.
F007 Quadrol Polyol, Batch No. WPYY-520B; produced Feb 04, 2003, purity
* unknown, stored at ambient temperature under nitrogen.
F020 904
EOR
F002 4
F010 2.2
F004 1
F005 ME
F006 The boiling point was deduced from vapor pressure data obtained by a
* dynamic method according to Directive 92/69/EEC, A.4.
F007 The boiling point was deduced from vapor pressure data obtained by a
* dynamic method according to Directive 92/69/EEC, A.4.
F020 827
EOR
F002 4
F010 2.2
F004 1
F005 RE
F006 BASF, Final Report, Physico-chemical properties of "Quadrol Polyol",
* Study No. 05L00061, GKA Competence Center Analytics, June, 2005.
F007 BASF, Final Report, Physico-chemical properties of "Quadrol Polyol",
* Study No. 05L00061, GKA Competence Center Analytics, June, 2005.
F020 400
EOR
F002 4
F010 2.2
F004 1
F005 RS
F006 At pressures above 50 hPa, temperatures decreased at constant pressures
* as a consequence of thermally caused changes in the test item. Therefore
* the normal boiling temperature could not be determined.
F007 At pressures above 50 hPa, temperatures decreased at constant pressures
* as a consequence of thermally caused changes in the test item. Therefore
* the normal boiling temperature could not be determined.
F020 870
EOR
F002 4
F010 2.2
F004 1
F005 TS
F006 Quadrol Polyol, Batch No. WPYY-520B, produced Feb 04, 2003, purity
* unknown, stored at ambient temperature under nitrogen.
F007 Quadrol Polyol, Batch No. WPYY-520B, produced Feb 04, 2003, purity
* unknown, stored at ambient temperature under nitrogen.
F020 905
EOR
F002 4
F010 2.3
F004 1
F005 RE
F006 MSDS, MDL Information Systems, 11 DEC 2001
F007 MSDS, MDL Information Systems, 11 DEC 2001

F020 401
 EOR
 F002 4
 F010 2.4
 F004 1
 F005 ME
 F006 MPBPWIN v1.41 (EPIWIN v3.11)
 F007 MPBPWIN v1.41 (EPIWIN v3.11)
 F020 402
 EOR
 F002 4
 F010 2.4
 F004 1
 F005 RL
 F006 calculated using scientifically acceptable method
 F007 calculated using scientifically acceptable method
 F020 667
 EOR
 F002 4
 F010 2.4
 F004 1
 F005 RM
 F006 Calculated in mm Hg, converted to hPa
 F007 Calculated in mm Hg, converted to hPa
 F020 726
 EOR
 F002 4
 F010 2.5
 F004 1
 F005 ME
 F006 KOWWIN v1.67 (EPIWIN v.3.11)
 F007 KOWWIN v1.67 (EPIWIN v.3.11)
 F020 403
 EOR
 F002 4
 F010 2.5
 F004 1
 F005 RL
 F006 calculated using scientifically acceptable method
 F007 calculated using scientifically acceptable method
 F020 666
 EOR
 F002 4
 F010 2.6.1
 F004 1
 F005 RE
 F006 Budavari, S., ed., The Merck Index: an encyclopedia of chemicals, drugs
 * and biologicals. 12th ed., Merck and Co., New Jersey, 1996.
 F007 Budavari, S., ed., The Merck Index: an encyclopedia of chemicals, drugs
 * and biologicals. 12th ed., Merck and Co., New Jersey, 1996.
 F020 664
 EOR
 F002 4
 F010 2.6.1
 F004 1
 F005 RL
 F006 Handbook data are assigned a reliability of 2


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F007 Handbook data are assigned a reliability of 2
F020 731
EOR
F002 4
F010 2.6.1
F004 1
F005 RM
F006 Quadrol is a base with pKa values of 4.30 and 8.99, respectively, for the
* two amine groups (McMahon, R., Brennan, M., and Glennon, J.D., Talanta
* 33(11):927 (1986).
F007 Quadrol is a base with pKa values of 4.30 and 8.99, respectively, for the
* two amine groups (McMahon, R., Brennan, M., and Glennon, J.D., Talanta
* 33(11):927 (1986).
F020 805
EOR
F002 4
F010 3.1.1
F004 1
F005 ME
F006 AOPWIN v1.91 (EPIWIN v3.11)
F007 AOPWIN v1.91 (EPIWIN v3.11)
F020 415
EOR
F002 4
F010 3.1.1
F004 1
F005 RL
F006 calculated using scientifically acceptable method
F007 calculated using scientifically acceptable method
F020 665
EOR
F002 4
F010 3.1.1
F004 1
F005 RS
F006
** AOP Program (v1.91) Results:
** =====
** SMILES : OC(C)CN(CCN(CC(O)C)CC(O)C)CC(O)C
** CHEM : 2-Propanol, 1,1',1'',1'''-(1,2-ethanediylldinitrilo)tetrakis-
** MOL FOR: C14 H32 N2 O4
** MOL WT : 292.42
** ----- SUMMARY (A
F007
** AOP Program (v1.91) Results:
** =====
** SMILES : OC(C)CN(CCN(CC(O)C)CC(O)C)CC(O)C
** CHEM : 2-Propanol, 1,1',1'',1'''-(1,2-ethanediylldinitrilo)tetrakis-
** MOL FOR: C14 H32 N2 O4
** MOL WT : 292.42
** ----- SUMMARY (AOP v1.91): HYDROXYL RADICALS -----
** Hydrogen Abstraction = 98.1801 E-12 cm3/molecule-sec
** Reaction with N, S and -OH = 132.5600 E-12 cm3/molecule-sec
** Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
** Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
** Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec
** Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

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**
**      OVERALL OH Rate Constant = 230.7401 E-12 cm3/molecule-sec
**      HALF-LIFE = .    0.046 Days (12-hr day; 1.5E6 OH/cm3)
**      HALF-LIFE = .    0.556 Hrs
**      ----- SUMMARY (AOP v1.91): OZONE REACTION -----
**
**      ***** NO OZONE REACTION. ESTIMATION *****
**      (ONLY Olefins and Acetylenes are Estimated)
**
**      Experimental Database: NO Structure Matches
**
F020 707
EOR
F002 4
F010 3.1.2
F004 2
F005 RM
F006 Due to the lack of hydrolyzable functional groups, Quadrol is expected to
* be stable to hydrolysis.
F007 Due to the lack of hydrolyzable functional groups, Quadrol is expected to
* be stable to hydrolysis.
F020 828
EOR
F002 4
F010 3.3.2
F004 1
F005 ME
F006 EPIWIN v3.11
F007 EPIWIN v3.11
F020 674
EOR
F002 4
F010 3.3.2
F004 1
F005 RL
F006 calculated using scientifically acceptable method
F007 calculated using scientifically acceptable method
F020 676
EOR
F002 4
F010 3.3.2
F004 1
F005 RS
F006
**      Level III Fugacity Model (Full-Output):
**      =====
**      Chem Name      : 2-Propanol,
*      1,1',1'',1'''-(1,2-ethanediyldinitrilo)tetrakis-
**      Molecular Wt: 292.42
**      Henry's LC   : 4.15e-016 atm-m3/mole (Henrywin program)
F007
**      Level III Fugacity Model (Full-Output):
**      =====
**      Chem Name      : 2-Propanol,
*      1,1',1'',1'''-(1,2-ethanediyldinitrilo)tetrakis-
**      Molecular Wt: 292.42

```

** Henry's LC : 4.15e-016 atm-m3/mole (Henrywin program)
 ** Vapor Press : 8.69e-009 mm Hg (Mpbpwin program)
 ** Liquid VP : 1.62e-007 mm Hg (super-cooled)
 ** Melting Pt : 154 deg C (Mpbpwin program)
 ** Log Kow : -2.08 (Kowwin program)
 ** Soil Koc : 0.00341 (calc by model)
 **

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	4.7e-008	1.11	1000
Water	49.8	900	1000
Soil	50.1	900	1000
Sediment	0.0918	3.6e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.42e-019	0.000693	1.11e-005	2.31e-005	3.71e-007
Water	8.37e-021	908	1.18e+003	30.3	39.3
Soil	3.11e-019	913	0	30.4	0
Sediment	7.71e-021	0.418	0.0435	0.0139	0.00145

** Persistence Time: 789 hr
 ** Reaction Time: 1.3e+003 hr
 ** Advection Time: 2.01e+003 hr
 ** Percent Reacted: 60.7
 ** Percent Advected: 39.3
 **

** Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
 ** Air: 1.113
 ** Water: 900
 ** Soil: 900
 ** Sediment: 3600
 ** Biowin estimate: 2.683 (weeks-months)
 **

** Advection Times (hr):
 ** Air: 100
 ** Water: 1000
 ** Sediment: 5e+004
 **

** -----
 * ----
 F020 677

EOR

F002 4

F010 3.5

F004 2

F005 RE

F006 BASF Corporation, 2005. Quadrol Polyol: Determination of the
 * Biodegradability in the DOC Die-Away Test, Laboratory Project No.
 * 21G0628/043373, May 2, 2005, Experimental Toxicology and Ecology, BASF
 * Aktiengesellschaft, 67056 Ludwigshafen/Rhe
 F007 BASF Corporation, 2005. Quadrol Polyol: Determination of the
 * Biodegradability in the DOC Die-Away Test, Laboratory Project No.
 * 21G0628/043373, May 2, 2005, Experimental Toxicology and Ecology, BASF

* Aktiengesellschaft, 67056 Ludwigshafen/Rhein, Germany.

F020 884

EOB

F002 4

F010 3.5

F004 2

F005 RS

F006 For the test substance, mean (N=2) DOC removal was 20% after 28 days and
* 41% after 42 days. For the reference substance, DOC removal was 91% after
* 14 days. The abiotic control indicated that elimination of the test
* substance by physico-chem

F007 For the test substance, mean (N=2) DOC removal was 20% after 28 days and
* 41% after 42 days. For the reference substance, DOC removal was 91% after
* 14 days. The abiotic control indicated that elimination of the test
* substance by physico-chemical processes was <10% at the end of exposure.
* The adsorption control indicated that only 5% of DOC was removed by
* adsorption. According to OECD criteria, the test substance is not readily
* biodegradable.

F020 887

EOB

F002 4

F010 3.5

F004 2

F005 TC

F006 The inoculum was non pre-adapted activated sludge from a laboratory
* wastewater plant treating municipal sewage, at a concentration of 30
* mg/L. The test duration was 42 days, consisting of 25 days in the
* adaptation phase and 17 days in the d

F007 The inoculum was non pre-adapted activated sludge from a laboratory
* wastewater plant treating municipal sewage, at a concentration of 30
* mg/L. The test duration was 42 days, consisting of 25 days in the
* adaptation phase and 17 days in the degradation phase.

F020 885

EOB

F002 4

F010 3.5

F004 2

F005 TS

F006 Quadrol Polyol, Batch No. WPYY-520B, 99.7% purity (BASF Proj. No. 66192),
* expiration date 31 July 2005, stored at room temperature under nitrogen.

F007 Quadrol Polyol, Batch No. WPYY-520B, 99.7% purity (BASF Proj. No. 66192);
* expiration date 31 July 2005, stored at room temperature under nitrogen.

F020 886

EOB

F002 4

F010 3.5

F004 3

F005 RE

F006 BASF Corporation, 2005. Quadrol Polyol: Determination of the Inhibition
* of Oxygen Consumption by Activated Sludge in the Activated Sludge
* Respiration Inhibition Test, Laboratory Project No. 08G0628/043374, April
* 13, 2005, Experimental Toxic

F007 BASF Corporation, 2005. Quadrol Polyol: Determination of the Inhibition
* of Oxygen Consumption by Activated Sludge in the Activated Sludge
* Respiration Inhibition Test, Laboratory Project No. 08G0628/043374, April
* 13, 2005, Experimental Toxicology and Ecology, BASF Aktiengesellschaft,
* 67056 Ludwigshafen/Rhein, Germany.

F020 888

EOR

F002 4

F010 3.5

F004 3

F005 RS

F006 There was no difference in oxygen consumption between the Quadrol-treated vessel and the blank controls. For inhibition of activated sludge respiration, the 30-minute EC20, EC50 and EC80 for Quadrol are all reported as >1000 mg/L (nominal).

F007 There was no difference in oxygen consumption between the Quadrol-treated vessel and the blank controls. For inhibition of activated sludge respiration, the 30-minute EC20, EC50 and EC80 for Quadrol are all reported as >1000 mg/L (nominal). Disturbances in the biodegradation process of activated sludge are not to be expected if the test substance is correctly introduced into adapted wastewater treatment plants at low concentrations. The test met the validity criteria, since the EC50 for the reference substance, 3,5-dichlorophenol, was about 7.5 mg/L and the deviation in the oxygen consumption in the blank controls was <15%.

F020 891

EOR

F002 4

F010 3.5

F004 3

F005 TC

F006 The inoculum was prepared from activated sludge from a laboratory wastewater plant treating municipal sewage. A concentration equivalent to 1 g/L of dry substance was used in the test. Test vessels contained synthetic medium and either test

F007 The inoculum was prepared from activated sludge from a laboratory wastewater plant treating municipal sewage. A concentration equivalent to 1 g/L of dry substance was used in the test. Test vessels contained synthetic medium and either test substance (1000 mg/L nominal) or reference substance (1, 10 or 100 mg/L dichlorophenol). Blank control vessels were not inoculated. Oxygen consumption rate was measured at intervals over a 30-minute period and changes compared to the blank control.

F020 890

EOR

F002 4

F010 3.5

F004 3

F005 TS

F006 Quadrol Polyol, Batch No. WPHY-520B, 99.7% purity (BASF Proj. No. 66192), expiration date 31 July 2005, stored at room temperature under nitrogen.

F007 Quadrol Polyol, Batch No. WPHY-520B, 99.7% purity (BASF Proj. No. 66192), expiration date 31 July 2005, stored at room temperature under nitrogen.

F020 889

EOR

F002 4

F010 4.1

F004 2

F005 ME

F006 Fathead minnows (35-50 mm length) were exposed to nominal concentrations of 0, 1.0, 10, 100 and 1000 ppm Quadrol using 10 fish per test concentration.

F007 Fathead minnows (35-50 mm length) were exposed to nominal concentrations

* of 0, 1.0, 10, 100 and 1000 ppm Quadrol using 10 fish per test
* concentration.

F020 734

EOR

F002 4

F010 4.1

F004 2

F005 RE

F006 Industrial Bio-Test Laboratories, Report No. 8560-08828, Four-Day Static
* Aquatic Toxicity Study with Quadrol in Fathead Minnows, May 4, 1976.

F007 Industrial Bio-Test Laboratories, Report No. 8560-08828, Four-Day Static
* Aquatic Toxicity Study with Quadrol in Fathead Minnows, May 4, 1976.

F020 733

EOR

F002 4

F010 4.1

F004 2

F005 RL

F006 Study pre-dates standardized methods and GLP. Basic data provided but
* test conditions not completely described.

F007 Study pre-dates standardized methods and GLP. Basic data provided but
* test conditions not completely described.

F020 732

EOR

F002 4

F010 4.1

F004 2

F005 RS

F006 No mortality was observed in any control or test concentration at any
* time during the study. No unusual behavioral reactions were noted among
* the exposed fish. Dissolved oxygen levels at 96 hours ranged from 5.2
* mg/L in the 100 ppm test con

F007 No mortality was observed in any control or test concentration at any
* time during the study. No unusual behavioral reactions were noted among
* the exposed fish. Dissolved oxygen levels at 96 hours ranged from 5.2
* mg/L in the 100 ppm test concentration to 6.4 mg/L in the control, while
* pH at 96 hours ranged from 7.2 in the control to 9.2 in the highest test
* concentration. The Litchfield-Wilcoxon method was used to calculate the
* TL-50.

F020 736

EOR

F002 4

F010 4.1

F004 2

F005 TC

F006 Tests were conducted in reconstituted water with pH 7.2-7.6, hardness
* 40-48 ppm calcium carbonate, and alkalinity of 30-35 ppm calcium
* carbonate. The test temperature was not reported; however, it was stated
* that the fish were held at 18 de

F007 Tests were conducted in reconstituted water with pH 7.2-7.6, hardness
* 40-48 ppm calcium carbonate, and alkalinity of 30-35 ppm calcium
* carbonate. The test temperature was not reported; however, it was stated
* that the fish were held at 18 degrees prior to testing. Dissolved oxygen
* and pH was measured in the control every 24 hours and in all test
* concentrations and control at 96 hours. A reference toxicant test was
* performed on the same lot of fish using p,p-DDT.

F020 735

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EOR
F002 4
F010 4.1
F004 2
F005 TS
F006 Test substance identified as Quadrol, but no information given about
* purity.
F007 Test substance identified as Quadrol, but no information given about
* purity.
F020 824
EOR
F002 4
F010 4.2
F004 1
F005 ME
F006 This estimate of the toxicity of Quadrol was made using ECOSAR v0.99g
* (EPWIN v3.11) using the SAR equation for the aliphatic amines class. The
* only input information was the CAS No. The octanol water partition
* coefficient was calculated using
F007 This estimate of the toxicity of Quadrol was made using ECOSAR v0.99g
* (EPWIN v3.11) using the SAR equation for the aliphatic amines class. The
* only input information was the CAS No. The octanol water partition
* coefficient was calculated using CLOGP, Ver. 3.3. The SAR equation used
* was Log 48-h LC50 (millimoles/L) = -0.524 - 0.584 logKow, where N=10,
*  $R^2=0.78$ , logKow<5.0, MW <1000
F020 416
EOR
F002 4
F010 4.2
F004 1
F005 RL
F006 calculated using scientifically acceptable method
F007 calculated using scientifically acceptable method
F020 681
EOR
F002 4
F010 4.2
F004 1
F005 RS
F006 ECOSAR Program (v0.99g) Results:
** =====
** SMILES : OC(C)CN(CCN(CC(O)C)CC(O)C)CC(O)C
** CHEM : 2-Propanol, 1,1',1'',1'''-(1,2-ethanediyldinitrilo)tetrakis-
** CAS Num: 000102-60-3
** ChemID1:
** ChemID2:
** ChemID3:
** M
F007 ECOSAR Program (v0.99g) Results:
** =====
** SMILES : OC(C)CN(CCN(CC(O)C)CC(O)C)CC(O)C
** CHEM : 2-Propanol, 1,1',1'',1'''-(1,2-ethanediyldinitrilo)tetrakis-
** CAS Num: 000102-60-3
** ChemID1:
** ChemID2:
** ChemID3:
** MOL FOR: C14 H32 N2 O4

```

** MOL WT : 292.42
 ** Log Kow: -2.08 (KowWin estimate)
 ** Melt Pt:
 ** Wat Sol: 1.886E+007 mg/L (calculated)
 **

** ECOSAR v0.99g Class(es) Found
 ** -----

** Aliphatic Amines
 **

ECOSAR Class	Predicted Organism	Duration	End Pt	mg/L (ppm)
Neutral Organic SAR 1.41e+006 (Baseline Toxicity)	: Fish	14-day	LC50	
Aliphatic Amines 32901.113	: Fish	96-hr	LC50	
Aliphatic Amines 1434.599	: Daphnid	48-hr	LC50	
Aliphatic Amines 661.806	: Green Algae	96-hr	EC50	
Aliphatic Amines 57.774	: Green Algae	96-hr	ChV	

** Note: * = asterick designates: Chemical may not be soluble
 ** enough to measure this predicted effect.
 ** Fish and daphnid acute toxicity log Kow cutoff: none
 ** Green algal EC50 toxicity log Kow cutoff: none
 ** Chronic toxicity log Kow cutoff: none
 ** MW cutoff: none
 **

** -----
 * -----
 F020 682

EOR

F002 4

F010 4.3

F004 1

F005 ME

F006 This estimate of the toxicity of Quadrol was made using ECOSAR v0.99g
 * (EPIWIN v3.11) using the SAR estimation for the aliphatic amine class.
 * The only input information was the CAS No. The octanol water partition
 * coefficient was calculated u

F007 This estimate of the toxicity of Quadrol was made using ECOSAR v0.99g
 * (EPIWIN v3.11) using the SAR estimation for the aliphatic amine class.
 * The only input information was the CAS No. The octanol water partition
 * coefficient was calculated using CLOGP, Ver. 3.3. The SAR equation used
 * to estimate the ChV was: $\text{Log ChV (millimoles/L)} = -1.399 - 0.334 \log \text{Kow}$,
 * where $N=11$, $R^2=0.61$, $\log \text{Kow} < 7.0$, $\text{MW} < 1000$. The SAR equation used to
 * estimate the 96-h EC50 was: $\text{Log } 96\text{-hEC50} = -0.548 - 0.434 \log \text{Kow}$

F020 417

EOR

F002 4


```
F010 4.3
F004 1
F005 RL
F006 calculated using scientifically acceptable method
F007 calculated using scientifically acceptable method
F020 683
EOR
F002 4
F010 4.3
F004 1
F005 RS
F006 ECOSAR Program (v0.99g) Results:
** =====
** SMILES : OC(C)CN(CCN(CC(O)C)CC(O)C)CC(O)C
** CHEM : 2-Propanol, 1,1',1'',1'''-(1,2-ethanediylldinitrilo)tetrakis-
** CAS Num: 000102-60-3
** ChemID1:
** ChemID2:
** ChemID3:
F007 ECOSAR Program (v0.99g) Results:
** =====
** SMILES : OC(C)CN(CCN(CC(O)C)CC(O)C)CC(O)C
** CHEM : 2-Propanol, 1,1',1'',1'''-(1,2-ethanediylldinitrilo)tetrakis-
** CAS Num: 000102-60-3
** ChemID1:
** ChemID2:
** ChemID3:
** MOL FOR: C14 H32 N2 O4
** MOL WT : 292.42
** Log Kow: -2.08 (KowWin estimate)
** Melt Pt:
** Wat Sol: 1.886E+007 mg/L (calculated)
**
** ECOSAR v0.99g Class(es) Found
** -----
** Aliphatic Amines
**
**
**
**
** Predicted
** ECOSAR Class Organism Duration End Pt mg/L
** (ppm)
** =====
** Neutral Organic SAR : Fish 14-day LC50
** 1.41e+006
** (Baseline Toxicity)
**
** Aliphatic Amines : Fish 96-hr LC50
** 32901.113
** Aliphatic Amines : Daphnid 48-hr LC50
** 1434.599
** Aliphatic Amines : Green Algae 96-hr EC50
** 661.806
** Aliphatic Amines : Green Algae 96-hr ChV
** 57.774
**
** Note: * = asterick designates: Chemical may not be soluble
```

** enough to measure this predicted effect.
** Fish and daphnid acute toxicity log Kow cutoff: none
** Green algal EC50 toxicity log Kow cutoff: none
** Chronic toxicity log Kow cutoff: none
** MW cutoff: none
**
**

**

*

F020 684

EOR

F002 4

F010 5.1.1

F004 1

F005 ME

F006 Doses prepared as 20% solution of Quadrol in water, neutralized to pH 7.

* Administered by stomach tube to male albino rats weighing approximately

* 100 grams. Animals observed for approximately one week following

* administration.

F007 Doses prepared as 20% solution of Quadrol in water, neutralized to pH 7.

* Administered by stomach tube to male albino rats weighing approximately

* 100 grams. Animals observed for approximately one week following

* administration.

F020 408

EOR

F002 4

F010 5.1.1

F004 1

F005 RE

F006 Hill Top Research Institute, Acute Oral Toxicity of Quadrol, March 7, 1956

F007 Hill Top Research Institute, Acute Oral Toxicity of Quadrol, March 7, 1956

F020 409

EOR

F002 4

F010 5.1.1

F004 1

F005 RL

F006 Study pre-dates GLPs and standardized methods. Basic documentation

* provided, details of methods lacking

F007 Study pre-dates GLPs and standardized methods. Basic documentation

* provided, details of methods lacking

F020 407

EOR

F002 4

F010 5.4

F004 2

F005 ME

F006 10 males and 10 females were used in each group (5 doses and untreated

* control). Doses were administered as 0.1%, 0.3%, 1%, 3% and 5% Quadrol in
* the feed. Body weight and feed consumption were determined weekly.

* Hematology parameters (hemog

F007 10 males and 10 females were used in each group (5 doses and untreated

* control). Doses were administered as 0.1%, 0.3%, 1%, 3% and 5% Quadrol in
* the feed. Body weight and feed consumption were determined weekly.

* Hematology parameters (hemoglobin concentration, erythrocyte counts,

* total white cell counts, and differential white cell counts) were

* determined at the initiation and termination of exposure. At termination,

* prothrombin time and organ weights (lungs, liver, spleen, kidneys,
* adrenal glands, gonads and pancreas), as well as liver fat, were
* determined.

F020 685

EOB

F002 4

F010 5.4

F004 2

F005 RE

F006 Hill Top Research Institute, Subacute Oral Toxicity of Quadrol, March 1,
* 1956, Project 151.

F007 Hill Top Research Institute, Subacute Oral Toxicity of Quadrol, March 1,
* 1956, Project 151.

F020 737

EOB

F002 4

F010 5.4

F004 2

F005 RL

F006 Study pre-dates GLPs and standardized methods. Basic documentation
* provided, details of methods lacking.

F007 Study pre-dates GLPs and standardized methods. Basic documentation
* provided, details of methods lacking.

F020 686

EOB

F002 4

F010 5.4

F004 2

F005 RS

F006 Animals in the two highest dose groups exhibited temporary decreased food
* consumption, loss of body weight, and interference with growth rate.
* After the first month, however, food intake and rate of growth was
* similar in all groups. Rats fed

F007 Animals in the two highest dose groups exhibited temporary decreased food
* consumption, loss of body weight, and interference with growth rate.
* After the first month, however, food intake and rate of growth was
* similar in all groups. Rats fed Quadrol at levels up to 1% of the diet
* (representing a dosage of 600 - 900 mg/kg/d) exhibited no signs of
* toxicity. Rats fed Quadrol at levels of 3% and 5% of the diet (reaching a
* maximum daily dose of 3300 mg/kg in the first week) suffered some failure
* to gain weight in the early weeks of the experiment, possibly due to
* unpalatability of the diet. In these higher dose groups no other evidence
* of toxicity was seen, except for a slightly greater incidence of
* borderline abnormalities of the liver, which were of questionable
* significance.

F020 687

EOB

F002 4

F010 5.5

F004 1

F005 RE

F006 Hachiya, N. and Takizawa, Y., Mutagenicity of Plastic Additives,
* Hen'igensei Shiken 3(3):147-154 (1994). Cited at
* <http://toxnet.nlm.nih.gov>, CCRIS Record number 8275, last updated
* 02/12/2001.

F007 Hachiya, N. and Takizawa, Y., Mutagenicity of Plastic Additives,
* Hen'igensei Shiken 3(3):147-154 (1994). Cited at

* <http://toxnet.nlm.nih.gov>, CCRIS Record number 8275, last updated
* 02/12/2001.

F020 414

EOR

F002 4

F010 5.5

F004 1

F005 RL

F006 secondary reference (from CCRIS in TOXNET)

F007 secondary reference (from CCRIS in TOXNET)

F020 413

EOB

C

X